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Equilibrium of fluid membranes endowed with orientational order

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Minimization of the low-temperature elastic free-energy functional of orientationally ordered membranes involves independent variation of the membrane-shape, while keeping the orientational order on it (its texture) fixed. We propose an operational, coordinate-independent method for implementing such a variation. Using the Nelson-Peliti formulation of elasticity that emphasizes the interplay between geometry, topology, and thermal fluctuations of orientationally ordered membranes, we minimize the elastic free energy to obtain equations governing their equilibrium shape, together with associated free boundary conditions. Our results are essential for understanding and predicting equilibrium shapes as well as textures of membranes and vesicles; particularly under conditions in which shape deformations are large.

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I. INTRODUCTION

Soft matter systems abound with lamellar fluids having in-plane orientational order. Nematic films, membranes, and vesicles with vector order, and cytoskeletal assemblies in cells belong to this category. The discovery of liquid crystalline smectic $L_{\beta'}$ phase of phospholipid membranes [1], and the feasibility of obtaining almost isolated, deformable membranes by hyperswelling it [2], motivated the exploration of the interplay between elasticity, topological defects, and thermal fluctuations in isolated fluid membranes with in-plane orientational order.

The remarkable interplay between the shape of a surface and frustration of the orientational order on it is familiar—a hairy ball cannot be combed flat without creating at least one hair-whorl or cowlick; a single vortex, or vortices, with total index 2 in the orientational order. The elegant spin-connection formulation of membrane elasticity by Nelson and Peliti [3] is particularly suited to the study of this interplay. It establishes that Gaussian curvature of membranes acts as a source of vortices—also known as disclinations—in the orientational order. Conversely, disclinations tend to bend flat, deformable membranes. These reciprocal effects help to mitigate the overall stress from bending of membranes, and that from deformations in the orientational order. Positive and negative disclinations of equal strength prefer locally positive (sphere-like) and negative (saddle-like) Gaussian curvatures, respectively, leading to asymmetry in their energies [4–6].

The interplay between shape and topological defects has been demonstrated in nematic and smectic vesicles [7]. Using colloidal, fluid membranes of finite lateral extent (i.e., with an edge or a boundary) [8], new methods for tuning the assembly and morphology of chiral molecules via control of interfacial tension [9], and edge tension [10] have now been developed. By photopatterning temperature-responsive polymer gel films, self-actuating materials that transform shape have been designed [11]. There has been recent theoretical work on obtaining cuboidal shapes using vesicles with tetratic

order [12]. In this context the problem of equilibrium shapes of membranes with free boundaries, addressed in this paper, gains special importance. We minimize the total, low-temperature free energy of orientationally ordered membranes with respect to variations in membrane-shape to obtain the covariant “shape equation”, together with free boundary conditions.

Our results are as follows. We give a precise, coordinate-independent, operational procedure for varying the membrane shape, while keeping the orientational order on it fixed (Fig. 1). We minimize the Nelson-Peliti elastic free energy Eq. (6) to obtain the first shape variation Eq. (35) that leads to the full shape Eq. (38) together with free boundary conditions Eq. (41). We derive the shape equation by using two different approaches. For the sake of simplicity, we do not treat anisotropic shape-order couplings that are specific to vector [13] and nematic [14] order in this paper. We obtain the exact solution of the coupled, nonlinear partial differential equations of equilibrium Eqs. (13) and (38) for a right-helical membrane to obtain the texture of orientational order on it, Eq. (61). Our solution has experimentally testable consequences for the energetics of dispirations (topological defects in smectic- C^* liquid crystals) [15]. Minimization of the elastic free energy Eq. (6) has been attempted earlier [16] within the conformal gauge. We point out the root cause of the erroneous results of Ref. [16]. We show that for membrane-configurations with nonzero mean curvature, our result leads to experimental consequences that are very different from those of Ref. [16].

This paper is organized as follows. Section II is a brief review of the Nelson-Peliti formulation. In Sec. III, we discuss the generalization of Lie dragging, which gives a purely geometric procedure for varying the membrane-shape without affecting the orientational order on it. In Sec. IV, we derive the shape equation from two different approaches. In Sec. IV A, we use the direct approach, which also yields free boundary conditions, whereas in Sec. IV B, we use the Coulomb gas version [4] of the Nelson-Peliti elastic free-energy to recover the result of Sec. IV A. This shows that our result is not dependent on the particular choice of gauge made in the direct method of Sec. IV A. In Sec. IV C we obtain the texture of orientational order on a helical membrane by solving the equations of equilibrium (the compatibility condition as

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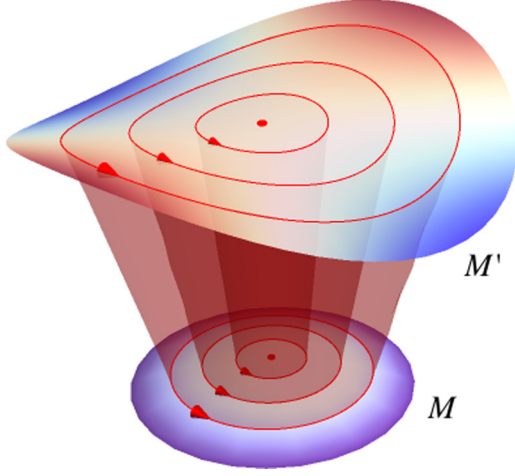


FIG. 1. Lie dragging the orientational order: Circular curves on the spherical, polar cap (the reference surface M) at the bottom are streamlines (integral curves) of the \hat{m} field that rotates through 2π upon traversing a closed loop enclosing the singular point; they correspond to a $+1$ disclination situated at the pole. The shape of M is varied (by an infinitesimal amount) to the saddle at the top (M'). The lightly shaded frustums of cones sandwiched between the surfaces have their apex at the center of M , so that the cones form loci of normals to streamlines on M . The streamlines on M' (which also correspond to a $+1$ disclination) are obtained by dragging the streamlines on M along the cones to the saddle. This ensures that there is no variation in the orientational order while implementing shape variation; the streamlines, and therefore the orientational order on the saddle is the same as that on the spherical cap.

well as the shape equation) exactly. We briefly discuss the experimental significance of this solution. In Sec. V we compare and contrast the shape Eq. (63) of Ref. [16] with our result Eq. (38), and we discuss experimental implications of these strikingly different results.

II. ELASTICITY OF FLUID MEMBRANES

A. Membranes without orientational order

In this section we briefly describe the well-known contributions to the free energy that are common to all fluid membranes, regardless of orientational order. The Helfrich free energy [17] of a deformable fluid membrane is

$$F_H = \int \left[\frac{\kappa}{2} (H - H_0)^2 + \kappa_G K \right] dS, \quad (1)$$

where H is the mean curvature, H_0 is the spontaneous curvature, K is the Gaussian curvature, κ, κ_G are elastic constants, and the integral is over the surface of the deformed membrane [18,19]. The spontaneous curvature $H_0 = 0$ for membranes with up-down symmetry. Gaussian curvature K is a total divergence. It does not contribute to the equations of equilibrium (the Euler-Lagrange equations) but contributes only to the boundary conditions.

The contribution to the total free energy from the surface tension σ of the membrane is

$$F_s = \sigma \int dS, \quad (2)$$

with $\sigma \geq 0$ for stability. The case $\sigma > 0$ is particularly important for tense fluid membranes [20].

For membranes with a boundary we have to include the edge free-energy,

$$F_e = \gamma \oint dl, \quad (3)$$

where γ is the coefficient of line tension, and the integral is over the boundary of the membrane.

There is a symmetry-allowed, anisotropic contribution to line tension that arises from the fact that the orientational order can prefer to have a particular orientation with respect to the outward normal to the membrane boundary. The nature of this contribution depends upon the symmetry of the orientational order (nematic or vector) [21,22]. Modifications to free boundary conditions due to anisotropic line tension will be discussed elsewhere [23].

For

$$\mathcal{F} = F_H + F_s + F_e, \quad (4)$$

the Euler-Lagrange equations together with free boundary conditions are known [24], and will be used in Sec. IV A to write the full shape equation, as well as the free boundary conditions.

B. Membranes with orientational order: The Nelson-Peliti formulation

In this section we consider the energetics of membranes with orientation order, and establish the notions and notation essential for what follows. The simplest continuum model with orientational order, the continuum xy model, has the low-temperature elastic free energy [25],

$$F_{xy} = \frac{k_s}{2} \int (\partial\theta)^2 dx dy, \quad (5)$$

where k_s is the spin-wave stiffness, the unit xy spin vector $\hat{m} = (\cos\theta, \sin\theta)$, and $\partial = (\partial_x, \partial_y)$ is the usual (flat space) gradient operator. We wish to generalize the flat-space xy model described above to spins on a deformable surface.

The generalization of Eq. (5) to spins on a deformable surface involves defining θ , as well as the appropriate “covariant derivative of θ ”, on a curved membrane. To define θ we set up a local, orthonormal frame $\hat{e}_i(\underline{\sigma})$, $i = \{1, 2\}$, in the tangent plane of the membrane, where $\underline{\sigma} = \sigma^\mu$ and $\mu = \{1, 2\}$ are internal coordinates on the membrane surface parametrized via the three-dimensional position vector $\mathbf{R}(\underline{\sigma})$. Thus, $\hat{m}(\underline{\sigma}) = (\cos\theta(\underline{\sigma}), \sin\theta(\underline{\sigma}))$ in the local Cartesian frame. The tangent vectors in the internal-coordinate basis are $\mathbf{t}_\mu(\underline{\sigma}) = \partial_\mu \mathbf{R}(\underline{\sigma}) = \partial \mathbf{R}(\underline{\sigma}) / \partial \sigma^\mu$. We reserve Greek letters for the indices of quantities represented in the coordinate (\mathbf{t}) basis, and Latin letters for those represented in the Cartesian (\hat{e}) basis. The \hat{e} basis is local; there is an $O(2)$ freedom in its choice—the tip of $\hat{e}_1(\underline{\sigma})$ can be placed at any point on the unit circle centered at $\underline{\sigma}$ and lying in the local tangent plane.

For deformable membranes the square-gradient elastic free energy Eq. (5) takes the form [3]

$$F_\theta = \frac{K_A}{2} \int (\mathcal{D}\theta)^2 dS = \frac{K_A}{2} \int (\partial\theta - \mathbf{A})^2 dS, \quad (6)$$

where we have introduced the notation $\mathcal{D}\theta = (\partial\theta - \mathbf{A})$, the “vector potential” \mathbf{A} is a local gauge field that corrects $\partial\theta$ so as to compensate for membrane curvature, and the integral is over the deformed membrane surface. \mathbf{A} is called the spin connection. The elastic free energy Eq. (6) is invariant under the local gauge transformation,

$$\theta \rightarrow \theta + \eta, \quad \mathbf{A} \rightarrow \mathbf{A} + \partial\eta. \quad (7)$$

The components

$$A_\mu = \frac{1}{2} \epsilon^{ij} (\partial_i \cdot \partial_\mu \partial_j), \quad (8)$$

where ϵ^{ij} is the totally antisymmetric unit symbol with $\epsilon^{12} = 1$.

The geometry of the membrane (represented by the Gaussian curvature K) and the topology of the θ field on it (represented by the disclination density \mathcal{S} , see below) are connected through [3]

$$\begin{aligned} \nabla \times \partial\theta &= \mathcal{S} \hat{\mathbf{n}}, \quad \text{and} \\ \nabla \times \mathbf{A} &= K \hat{\mathbf{n}}, \end{aligned} \quad (9)$$

where ∇ represents the covariant gradient operator, and $\hat{\mathbf{n}} = (\mathbf{t}_1 \times \mathbf{t}_2)/|\mathbf{t}_1 \times \mathbf{t}_2|$ is the unit normal to the membrane. The disclination density

$$\mathcal{S}(\underline{\sigma}) = \frac{2\pi}{\sqrt{g}} \sum_m q_m \delta^{(2)}(\underline{\sigma} - \tilde{\underline{\sigma}}_m), \quad (10)$$

with discrete disclination charges q_m located at $\tilde{\underline{\sigma}}_m$. In Eq. (10) above, g is the determinant of the metric tensor $g_{\mu\nu} = \mathbf{t}_\mu \cdot \mathbf{t}_\nu$, and $\delta^{(2)}(\underline{\sigma} - \tilde{\underline{\sigma}}_m)$ is the two-dimensional Dirac δ . The Gaussian curvature $K = \text{Det}[K_\mu^\nu]$ is the determinant of the curvature tensor $K_{\mu\nu} = \hat{\mathbf{n}} \cdot \partial_\mu \mathbf{t}_\nu$. The importance of the relations Eqs. (9) is brought out by the compatibility condition discussed in Sec. II C below.

C. Equilibrium of membranes

1. The compatibility condition

We now consider the equation of equilibrium for F_θ obtained by varying θ while keeping the membrane shape fixed [4]:

$$\frac{\delta F_\theta}{\delta \theta} = -K_A \nabla \cdot \mathcal{D}\theta = 0. \quad (11)$$

The Airy stress function χ defined by

$$\mathcal{D}^\mu \theta = \gamma^{\mu\nu} \partial_\nu \chi \quad (12)$$

identically satisfies $\delta F_\theta / \delta \theta = 0$, where the covariant version of the unit antisymmetric tensor $\gamma^{\mu\nu} = \epsilon^{\mu\nu} / \sqrt{g}$. However, χ has to obey the condition

$$\nabla^2 \chi = K - \mathcal{S}, \quad (13)$$

which ensures compatibility between the shape of the membrane and topology of the orientational order embedded in it.

The variational problem of minimizing F_θ also yields the free boundary condition for membranes with a boundary,

$$n_{(b)}^\mu \gamma_{\mu\nu} \partial^\nu \chi = 0, \quad (14)$$

where $\hat{\mathbf{n}}_{(b)}$ is the unit outward normal to the boundary.

2. The shape equation: Small deformations

In the Monge gauge, the membrane is parametrized in terms of a “height field” $f(x, y)$ in Cartesian coordinates, and the approximate expressions (small deformations) for mean, and Gaussian curvatures are $H \simeq (1/2)\nabla^2 f$ and $K \simeq \epsilon_{ij}\epsilon_{kl}(\partial_i \partial_k f)(\partial_j \partial_l f)$, respectively, where the Laplacian operator $\nabla^2 = \partial_x^2 + \partial_y^2$. Within this approximation the minimization of $F_H + F_\theta$ with respect to the height field f gives [4]

$$\frac{\tilde{\kappa}}{K_A} \nabla^4 f = (\partial_y^2 \chi)(\partial_x^2 f) + (\partial_x^2 \chi)(\partial_y^2 f) - 2(\partial_x \partial_y \chi)(\partial_x \partial_y f), \quad (15)$$

where $\tilde{\kappa} = \kappa/4$. This equation, called the “nonlinear, hexatic von Kármán equation” is valid for small deformations of the membrane shape. In deriving this equation it is assumed that the membrane-shape can be varied without affecting the orientational order on it.

The compatibility condition Eq. (13) and the shape Eq. (15) constitute the coupled, nonlinear partial differential equations of equilibrium.

III. INDEPENDENT VARIATION OF SHAPE: LIE DRAGGING

To vary the shape $\mathbf{R}(\underline{\sigma})$ of the membrane while keeping the θ field fixed, we set

$$\delta \mathbf{R} = \mathbf{t}_\mu \delta R_\parallel^\mu + \hat{\mathbf{n}} \delta R_\perp, \quad (16)$$

where δR_\parallel and δR_\perp are, respectively, the variations in the tangent plane of the membrane, and along its normal. In carrying out shape variation δR_\perp , we need to ensure that $\delta\theta = 0$ for arbitrary, nonzero δR_\perp . It is not obvious how the membrane shape can be varied without affecting the orientational order on it. Earlier work on shape variation of membranes [4,16] implicitly assumes that such a variation can be carried out, without pointing out how it is to be implemented. In what follows we propose a coordinate-independent (purely geometric), operational procedure for effectuating independent shape variation by generalizing the concept of Lie dragging [26] to vector fields (Fig. 1).

Let us consider the reference configuration M of a membrane whose shape we wish to vary by an infinitesimal amount to the target configuration M' . The $\hat{\mathbf{m}}$ field on M can be represented by streamlines, also called integral curves, defined so that the unit tangent at any point on the integral curve gives $\hat{\mathbf{m}}$ at that point. Consider two nearby points, $\mathbf{R}(\underline{\sigma})$ and $\mathbf{R}(\underline{\sigma} + d\underline{\sigma})$, which are connected by $\hat{\mathbf{m}}$ on its integral curve in the reference membrane M . Upon shape variation to a configuration M' along the normal to M ,

$$\mathbf{R}'(\underline{\sigma}) = \mathbf{R}(\underline{\sigma}) + \hat{\mathbf{n}}(\underline{\sigma}) \delta R_\perp(\underline{\sigma}), \quad (17)$$

and

$$\mathbf{R}'(\underline{\sigma} + d\underline{\sigma}) = \mathbf{R}(\underline{\sigma} + d\underline{\sigma}) + \hat{\mathbf{n}}(\underline{\sigma} + d\underline{\sigma}) \delta R_\perp(\underline{\sigma} + d\underline{\sigma}). \quad (18)$$

For sufficiently small shape variations δR_\perp , the normals of points on the integral curve do not intersect; they are said to form a congruence. The vector $\hat{\mathbf{m}}'$ connecting the points $\mathbf{R}'(\underline{\sigma})$ and $\mathbf{R}'(\underline{\sigma} + d\underline{\sigma})$ on M' is the Lie dragged version of $\hat{\mathbf{m}}$ on

M . Lie dragging all the integral curves on M in this manner transfers the entire $\hat{\mathbf{m}}$ field to the varied surface M' .

In Fig. 1 we illustrate the idea of keeping the orientational order on the membrane fixed, despite variation in membrane-shape. We use a particularly simple example that nevertheless emphasizes the fact that fields with disclinations can also be Lie dragged without any ambiguity by excising the singular, disclination points from M .

IV. THE SHAPE EQUATION: LARGE DEFORMATION

In this section we derive the shape equation for large deformations by two methods. The first method directly uses the free energy Eq. (6) with a particular choice of gauge, whereas the second method uses the Coulomb gas representation of Eq. (6) (see below). Derivation of the shape equation by the second method is necessary to show that the result obtained via the direct method does not depend on the particular choice of gauge made in the first method. These two methods are complementary—apart from the shape equation, the first method also gives free boundary conditions, which the second method cannot.

A. Shape variation I: Direct method

To obtain the first variation of Eq. (6) with respect to shape we first write it in its full, covariant form:

$$F_\theta = \frac{K_A}{2} \int (\partial_\mu \theta - A_\mu) g^{\mu\nu} (\partial_\nu \theta - A_\nu) \sqrt{g} d\sigma^1 d\sigma^2. \quad (19)$$

The shape variations of $g^{\mu\nu}$ and \sqrt{g} are well-known [see Eqs. (33) and (34) below]. Thus, we need to evaluate

$$\delta A_\mu = \frac{1}{2} \epsilon^{ij} \delta(\hat{\mathbf{e}}_i \cdot \partial_\mu \hat{\mathbf{e}}_j). \quad (20)$$

To this end, we first obtain $\delta \mathbf{e}_k$ in the \mathbf{t} and $\hat{\mathbf{e}}$ bases. A comparison of the results of the variation, followed by a judicious choice of gauge leads to the shape variation.

The Cartesian basis $\hat{\mathbf{e}}_i$ can be expanded in the basis of local tangent vectors $\mathbf{t}_\mu = \partial_\mu \mathbf{R}$, so that

$$\hat{\mathbf{e}}_i = E_i^\mu \mathbf{t}_\mu, \quad (21)$$

where components of E_i^μ form a 2×2 invertible matrix, called the *vierbein* (“four legs” in German). Using the known result for the variation of tangent vectors,

$$\delta \mathbf{t}_\mu = \delta U_\mu^\nu \mathbf{t}_\nu + \delta V_\mu \hat{\mathbf{n}}, \quad (22)$$

with

$$\delta U_\mu^\nu = \nabla_\mu \delta R_\parallel^\nu - K_\mu^\nu \delta R_\perp, \text{ and} \quad (23)$$

$$\delta V_\mu = K_{\mu\nu} \delta R_\parallel^\nu + \nabla_\mu \delta R_\perp, \quad (24)$$

where the curvature tensor $K_{\mu\nu} = \hat{\mathbf{n}} \cdot \partial_\mu \mathbf{t}_\nu$, we get

$$\delta \mathbf{e}_k = (\delta E_k^\mu + E_k^\nu \delta U_\nu^\mu) \mathbf{t}_\mu + E_k^\mu \delta V_\mu \hat{\mathbf{n}} \quad (25)$$

in the \mathbf{t} basis.

The variation $\delta \mathbf{e}_k$ has the form

$$\delta \mathbf{e}_k(\sigma) = \epsilon_k^l \hat{\mathbf{e}}_l(\sigma) \delta_\parallel(\sigma) + \hat{\mathbf{n}}(\sigma) \delta_\perp(\sigma) \quad (26)$$

in the $\hat{\mathbf{e}}$ basis, where $\delta_\parallel, \delta_\perp(\sigma)$ are small variations. The term $\epsilon_k^l \hat{\mathbf{e}}_l(\sigma) \delta_\parallel(\sigma)$ corresponds to infinitesimal, anticlockwise

rotation of the $\hat{\mathbf{e}}$ basis and reflects the local $O(2)$ gauge freedom.

Next, we fix the gauge by setting $\delta_\parallel(\sigma) = 0$. One way of ensuring this is by excising all disclination points from the membrane and positing $\hat{\mathbf{e}}_1(\sigma) \parallel \hat{\mathbf{m}}(\sigma)$ on local, overlapping patches covering the reference surface M , thus securing $\theta(\sigma) = 0$ locally. The integral curves of $\hat{\mathbf{e}}_1$ on M are then identical to those of $\hat{\mathbf{m}}$, and implementing the variation $\delta \mathbf{e}_k$ amounts to Lie dragging the $\hat{\mathbf{m}}$ field from M to M' [see Eq. (26) above in conjunction with Eqs. (17) and (18)]. With this choice of gauge, a comparison of the expressions for $\delta \mathbf{e}_k$ in the two bases, Eqs. (25) and (26), gives

$$\delta E_k^\mu = -E_k^\nu \delta U_\nu^\mu, \text{ and } \delta \mathbf{e}_k = E_k^\mu \delta V_\mu \hat{\mathbf{n}}. \quad (27)$$

Using the standard definitions,

$$K_{\mu\nu} = \hat{\mathbf{n}} \cdot \partial_\mu \mathbf{t}_\nu; \quad \partial_\mu \hat{\mathbf{n}} = -K_{\mu\nu} \mathbf{t}^\nu, \quad (28)$$

and substituting for $\delta \mathbf{e}_k$ from Eq. (27), we get

$$\delta A_\mu = \epsilon^{ij} E_i^\alpha \delta V_\alpha E_j^\sigma K_{\sigma\mu}, \quad (29)$$

which we simplify below.

To derive the shape variation $(\delta F_\theta / \delta R_\perp)$ we first exploit the orthonormality of the $\hat{\mathbf{e}}$ basis, which gives the relation $E^{\alpha i} E_i^\sigma = g^{\alpha\sigma}$ for the *vierbein*. This in turn implies that

$$\epsilon^{ij} E_i^\alpha E_j^\sigma = \frac{\epsilon^{\alpha\sigma}}{\sqrt{g}} = \gamma^{\alpha\sigma}, \quad (30)$$

which is the contravariant version of the unit antisymmetric symbol. Equation (30) above can be inferred by noticing that

$$(\epsilon^{ij} E_i^\alpha E_j^\sigma) (\epsilon^{kl} E_k^\mu E_l^\nu) = g^{\alpha\mu} g^{\sigma\nu} - g^{\alpha\nu} g^{\sigma\mu}. \quad (31)$$

Next, we use Eqs. (24) and (30) to simplify Eq. (29), and we get

$$\delta A_\mu = \gamma^{\alpha\sigma} K_{\sigma\mu} (\nabla_\alpha \delta R_\perp + K_{\alpha\nu} \delta R_\parallel^\nu), \quad (32)$$

which expresses δA solely in terms of the internal coordinates of the membrane. Finally, we use the known variations

$$\delta g_{\mu\nu} = \nabla_\mu \delta R_\parallel^\nu + \nabla_\nu \delta R_\parallel^\mu - 2K_{\mu\nu} \delta R_\perp, \quad (33)$$

and

$$\delta \sqrt{g} = \sqrt{g} \nabla_\mu \delta R_\parallel^\mu - 2H \sqrt{g} \delta R_\perp, \quad (34)$$

together with the definition of the Airy stress function (12) to obtain

$$\frac{\delta F_\theta}{\delta R_\perp} = K_A (K^{\mu\nu} \Psi_{\mu\nu} + H \Phi), \quad (35)$$

where $H = (1/2) K_\mu^\mu$ is the mean curvature, and we have defined

$$\Psi_{\mu\nu} = \nabla_\mu \nabla_\nu \chi - (\nabla_\mu \chi)(\nabla_\nu \chi), \quad (36)$$

$$\Phi = (\nabla \chi)^2 - 2 \nabla^2 \chi. \quad (37)$$

In writing Eq. (35), the term $K_A (\gamma_{\mu\nu} \partial^\nu \chi) (\gamma^{\alpha\beta} \nabla_\alpha K_\beta^\mu)$ obtained in performing the variation has been discarded, assuming nonsingular parametrization of membrane patches, so that $\gamma^{\alpha\beta} \nabla_\alpha K_\beta^\mu = 0$.

A natural question that arises at this stage is whether the result Eq. (35) depends upon the particular choice of gauge $\delta_{||}(\underline{\sigma}) = 0$. In Sec. IV B we derive Eq. (35) starting from the Coulomb gas model of the elastic free energy F_θ . This calculation does not involve fixing the gauge, and recovers the result Eq. (35), thus demonstrating that Eq. (35) does not depend on the choice of gauge.

As stated in Sec. II A, the Euler-Lagrange equations together with free boundary conditions for $\mathcal{F} = F_H + F_s + F_e$ are known [24]. For the sake of completeness and convenience, we explicitly write the full shape equation for the total free energy $\mathcal{F} = \mathcal{F} + F_\theta$,

$$\frac{\delta F_\theta}{\delta R_\perp} + \frac{\delta \mathcal{F}}{\delta R_\perp} = 0, \quad (38)$$

where the first term is given by Eq. (35) and where

$$\frac{\delta \mathcal{F}}{\delta R_\perp} = \frac{\kappa}{2} [\nabla^2 H + 2(H - H_0)(H^2 - K + HH_0)] - 2\sigma H. \quad (39)$$

We note that the shape Eq. (38) simplifies considerably for minimal surfaces (those with mean curvature $H = 0$). To the lowest order, and for spontaneous curvature $H_0 = 0$, Eq. (38) reduces to the von Kármán Eq. (15) of Sec. II C 2. The compatibility condition Eq. (13) and the shape Eq. (38) form the pair of coupled, nonlinear partial differential equations of bulk equilibrium.

To obtain the contribution of F_θ to free boundary conditions resulting from shape variation, we follow the methods of Ref. [24]. A distinctive feature of this variational problem is that the boundary conditions are prescribed on a curve that is initially unspecified, and the shape of bounding curve itself has to be deduced in solving the problem. Describing the boundary curve in the arc-length parametrization $\mathbf{R}(s)$, and using the unit triad (also called the Darboux frame) comprising the unit tangent to the boundary $\hat{\mathbf{t}}_{(b)}(s) = d\mathbf{R}(s)/ds$, the surface normal at the boundary $\hat{\mathbf{n}}(s)$, and the *outward* normal to the boundary $\hat{\mathbf{n}}_{(b)}(s) = \hat{\mathbf{t}}_{(b)}(s) \times \hat{\mathbf{n}}(s)$, we employ the following notation:

$$\begin{aligned} \nabla_{||} &= \mathbf{t}_{(b)}^\mu \nabla_\mu, \quad \nabla_\perp = \mathbf{n}_{(b)}^\mu \nabla_\mu, \quad K_{||} = \mathbf{t}_{(b)}^\mu \mathbf{t}_{(b)}^\nu K_{\mu\nu}, \\ K_\perp &= \mathbf{n}_{(b)}^\mu \mathbf{n}_{(b)}^\nu K_{\mu\nu}, \text{ and } K_{||\perp} = \mathbf{t}_{(b)}^\mu \mathbf{n}_{(b)}^\nu K_{\mu\nu}. \end{aligned} \quad (40)$$

The free boundary conditions from shape variation of the total free energy $\mathcal{F} = \mathcal{F} + F_\theta$, corresponding, respectively, to variations along $\hat{\mathbf{n}}_{(b)}$, $\hat{\mathbf{n}}$, and $\hat{\mathbf{t}}_{(b)}$, are

$$\begin{aligned} K_A[(\nabla\chi)^2 + (\nabla_{||}\chi)^2] + \hat{\mathbf{n}}_{(b)} \cdot (\delta\mathcal{F}/\delta\mathbf{R})|_{\partial M} &= 0, \\ K_A(\nabla_\perp\chi) K_{||} + \hat{\mathbf{n}} \cdot (\delta\mathcal{F}/\delta\mathbf{R})|_{\partial M} &= 0, \quad \text{and} \\ \hat{\mathbf{t}}_{(b)} \cdot (\delta\mathcal{F}/\delta\mathbf{R})|_{\partial M} &= 0, \end{aligned} \quad (41)$$

where the boundary contributions from the variation of \mathcal{F} are [24]

$$\begin{aligned} \hat{\mathbf{n}}_{(b)} \cdot \frac{\delta\mathcal{F}}{\delta\mathbf{R}} \Big|_{\partial M} &= \kappa(H - H_0)^2 + 2(\kappa_G K + \gamma k_g + \sigma), \\ \hat{\mathbf{n}} \cdot \frac{\delta\mathcal{F}}{\delta\mathbf{R}} \Big|_{\partial M} &= \frac{\kappa}{2} \nabla_\perp H - \kappa_G \nabla_{||} K_{||\perp} + \gamma K_{||}, \text{ and} \\ \hat{\mathbf{t}}_{(b)} \cdot \frac{\delta\mathcal{F}}{\delta\mathbf{R}} \Big|_{\partial M} &= \frac{\kappa}{2} H + \kappa_G K_{||}. \end{aligned} \quad (42)$$

In the first of Eqs. (42), k_g is the geodesic curvature of the bounding curve. Note that in Eq. (41), $\gamma_{\mu\nu} \nabla^\nu \chi = \mathcal{D}_\mu \theta$. Thus, Eqs. (14) and (41) constitute the full set of free boundary conditions. For minimal surfaces, the boundary conditions simplify considerably.

B. Shape variation II: Coulomb-gas model

In this section we obtain the shape equation by using the Coulomb-gas representation of F_θ [see Eq. (50) below], as in Ref. [16]. This has twofold advantages: we can (i) check that the result of Sec. IV A is independent of the particular choice of gauge $\delta_{||}(\underline{\sigma}) = 0$, and (ii) directly compare our result with that of Ref. [16]. Reference [16] uses the conformal gauge, with the restriction that the disclination density $\mathcal{S} = 0$. We do not confine ourselves to the restriction $\mathcal{S} = 0$, and use a general gauge. It is instructive to derive the Coulomb gas representation Eq. (50), particularly because some concepts and relations that appear as intermediate steps in deriving it are useful in obtaining the final result.

The compatibility condition Eq. (13),

$$\nabla^2 \chi(\underline{\sigma}) = K(\underline{\sigma}) - \mathcal{S}(\underline{\sigma}) = \rho(\underline{\sigma}), \quad (43)$$

is the Poisson equation in two-dimensions, with $\rho(\underline{\sigma})$ as the source. To solve for $\chi(\underline{\sigma})$, we define the Green's function for an unbounded membrane of infinite extent by

$$\nabla_{\underline{\sigma}}^2 G(\underline{\sigma}, \underline{\sigma}') = \frac{\delta^{(2)}(\underline{\sigma}, \underline{\sigma}')}{\sqrt{g(\underline{\sigma}')}}, \quad (44)$$

where $\nabla_{\underline{\sigma}}^2$ is the Laplacian operator in the metric $g_{\mu\nu}(\underline{\sigma})$, and $\delta^{(2)}(\underline{\sigma}, \underline{\sigma}')$ is the two-dimensional Dirac δ . The solution,

$$\chi(\underline{\sigma}) = \int G(\underline{\sigma}, \underline{\sigma}') \rho(\underline{\sigma}') \sqrt{g(\underline{\sigma}')} d^2\sigma', \quad (45)$$

implies that

$$\nabla_\mu \chi(\underline{\sigma}) = \int [\nabla_\mu G(\underline{\sigma}, \underline{\sigma}')] \rho(\underline{\sigma}') \sqrt{g(\underline{\sigma}')} d^2\sigma', \quad (46)$$

where ∇_μ refers to the gradient operator in unprimed coordinates. Recalling the definition Eq. (12) for the Airy stress function χ , and using the explicit form of the square-gradient elasticity Eq. (19), we get

$$F_\theta = \frac{K_A}{2} \int (\nabla_\mu \chi)(\nabla^\mu \chi) \sqrt{g} d^2\sigma. \quad (47)$$

Substituting the expression for $\nabla_\mu \chi$ from Eq. (46), integrating over $d^2\sigma$ by parts, and ignoring the boundary term (on the grounds that the Green's function is here defined for an unbounded, infinite membrane), we get

$$F_\theta = -\frac{K_A}{2} \iint \rho(\underline{\sigma}') \mathcal{G}(\underline{\sigma}', \underline{\sigma}'') \rho(\underline{\sigma}'') dS' dS'', \quad (48)$$

where $dS' = \sqrt{g(\underline{\sigma}')} d^2\sigma'$, $dS'' = \sqrt{g(\underline{\sigma}'')} d^2\sigma''$ are area elements, and

$$\mathcal{G}(\underline{\sigma}', \underline{\sigma}'') = \int G(\underline{\sigma}, \underline{\sigma}') \nabla_{\underline{\sigma}}^2 G(\underline{\sigma}, \underline{\sigma}'') \sqrt{g(\underline{\sigma}')} d^2\sigma. \quad (49)$$

Using the defining relation Eq. (44) for the Green's function, and integrating Eq. (48) over $d^2\sigma''$, we get the Coulomb-gas

model [4],

$$F_\theta = -\frac{K_A}{2} \iint \rho(\underline{\sigma}) G(\underline{\sigma}, \underline{\sigma}') \rho(\underline{\sigma}') dS dS', \quad (50)$$

where $\rho(\underline{\sigma}) = K(\underline{\sigma}) - \mathcal{S}(\underline{\sigma})$.

It is convenient to use the abbreviated notation $\rho(\underline{\sigma}) = \rho$, $\rho(\underline{\sigma}') = \rho'$, $g(\underline{\sigma}) = g$, $g(\underline{\sigma}') = g'$ and $G(\underline{\sigma}, \underline{\sigma}') = G$. The shape variation is

$$\begin{aligned} \delta F_\theta &= -K_A \iint \rho' [G \delta(\rho \sqrt{g}) + (\delta G) \rho \sqrt{g}] d^2 \sigma \sqrt{g'} d^2 \sigma' \\ &= (\delta F_\theta^{(1)} + \delta F_\theta^{(2)}), \end{aligned} \quad (51)$$

where the second line retains the ordering of terms in the first line.

To calculate $\delta F_\theta^{(1)}$ of Eq. (51) we need the variation $\delta \rho = \delta K - \delta \mathcal{S}$. We note that in evaluating $\delta \mathcal{S}$, the disclination density is to be interpreted in a coarse-grained sense, so that \mathcal{S} is, formally, the disclination density corresponding to a continuous distribution of disclinations. It is straightforward to obtain

$$\delta \mathcal{S} = 2H \mathcal{S} \delta R_\perp. \quad (52)$$

To evaluate δK we use the Gauss-Codazzi relation,

$$K_{\mu\alpha} K^\alpha_\nu = 2H K_{\mu\nu} - K g_{\mu\nu}, \quad (53)$$

which leads to

$$\delta K = 2H \nabla^2 \delta R_\perp - K_{\mu\nu} \nabla^\nu \nabla^\mu \delta R_\perp + 2H K \delta R_\perp. \quad (54)$$

Using $\delta \sqrt{g} = -2H \sqrt{g} \delta R_\perp$ Eq. (34) for the normal variation, it is straightforward to simplify $\delta(\rho \sqrt{g})$. Integrating $\delta F_\theta^{(1)}$ by parts, ignoring boundary contributions, and using Eq. (45) to cast the result in terms of the stress function χ , we have

$$\delta F_\theta^{(1)} = K_A \int (K_{\mu\nu} \nabla^\nu \nabla^\mu \chi - 2H \nabla^2 \chi) \delta R_\perp dS. \quad (55)$$

It is noteworthy that terms involving \mathcal{S} cancel off in the calculation of $\delta F_\theta^{(1)}$.

The evaluation of $\delta F_\theta^{(2)}$ is more involved. First, we vary Eq. (44) to get

$$\delta \nabla^2 G(\underline{\sigma}, \underline{\sigma}') = -\frac{\delta^{(2)}(\underline{\sigma}, \underline{\sigma}')}{2g(\underline{\sigma}')} \delta \sqrt{g(\underline{\sigma}')}, \quad (56)$$

where

$$\nabla^2 G = (1/\sqrt{g}) \partial_\mu (\sqrt{g} g^{\mu\nu} \partial_\nu G) \quad (57)$$

is the explicit form of the Laplacian. Next, we use the relations $\delta g^{\mu\nu} = 2K^{\mu\nu} \sqrt{g} \delta R_\perp$ and $\delta \sqrt{g} = -2H \sqrt{g} \delta R_\perp$ for normal variations [see Eqs. (33) and (34)], to obtain

$$\nabla^2 \delta G = \frac{1}{\sqrt{g}} \partial_\mu [\sqrt{g} (H g^{\mu\nu} - K^{\mu\nu}) (\partial_\nu G) \delta R_\perp]. \quad (58)$$

Equation (58) above implies that

$$\nabla^\mu \delta G = (H g^{\mu\nu} - K^{\mu\nu}) (\partial_\nu G) \delta R_\perp, \quad (59)$$

apart from the curl of a well-behaved vector field. Finally, using Eq. (59) in conjunction with the compatibility condition

Eq. (43), its solution Eq. (45), and integrating by parts, we get

$$\delta F_\theta^{(2)} = K_A \int [H (\nabla \chi)^2 - (\nabla^\mu \chi) K_\mu^\nu (\nabla_\nu \chi)] \delta R_\perp \sqrt{g} dS. \quad (60)$$

Adding up the contributions $\delta F_\theta^{(1)}$ and $\delta F_\theta^{(2)}$, we recover the result Eq. (35) of Sec. IV A.

C. Solution for a helicoid

The coupled equations of bulk equilibrium, Eqs. (13) and (38), can be solved for the texture on a right-helicoidal membrane (the shape of the membrane is prescribed to be a right-helicoid). For a right-helicoid of pitch p , parametrized by the position vector $\mathbf{R} = (\rho \cos \phi, \rho \sin \phi, \tilde{p} \phi)$, where ρ and ϕ are internal coordinates, $\tilde{p} = p/(2\pi)$; the components of the metric tensor are $g_{\rho\rho} = 1$, $g_{\rho\phi} = g_{\phi\rho} = 0$, $g_{\phi\phi} = \rho^2 + \tilde{p}^2$, the determinant of the metric $g = \rho^2 + \tilde{p}^2$, the curvature tensor has components $K_{\rho\rho} = K_{\phi\phi} = 0$, $K_{\rho\phi} = K_{\phi\rho} = -\tilde{p}/\sqrt{g}$, the mean curvature $H = 0$ (the helicoid is a minimal surface), the Gaussian curvature $K = -\tilde{p}^2/g^2$, and the components of spin-connection are $(A_\rho, A_\phi) = (0, -\rho/\sqrt{g})$. Using these geometrical attributes of a helicoid we find that the solution is

$$\begin{aligned} \chi &= \frac{\alpha}{2\pi} \ln(\rho + \sqrt{\rho^2 + \tilde{p}^2}) - \frac{1}{2} \ln(\rho^2 + \tilde{p}^2) + \beta \\ \implies \theta &= \alpha \phi + \beta, \end{aligned} \quad (61)$$

where α, β are arbitrary constants. We emphasize that the solution obtained above is an exact solution to the compatibility condition *as well as the shape equation*. It has been obtained by assuming that the membrane is free of disclinations. In a previous publication that extends the Nelson-Peliti formulation to smectic liquid crystals with in-plane orientational order [15], we have used this solution to demonstrate dispersion asymmetry in chiral smectic-C* liquid crystals. Dispersions with indices of the same magnitude but opposite signs have disparate energies—a result that is amenable to experimental tests.

V. DISCUSSION

In this section we first briefly consider the nature of the equations of equilibrium for membranes with orientational order. This is followed by an appraisal of the results of Ref. [16]. Finally, we discuss experimental situations where our results would lead to vastly different results from those of Ref. [16].

The coupled, nonlinear partial differential equations of equilibrium, Eqs. (13) and (38), are covariant, fluid-membrane analogues of the Föppl-von Kármán equations for large deflections of thin plates [27] modified to account for topological defects [28]. As is the case for thin-plate equations, “These equations are very complicated, and cannot be solved exactly, even in very simple cases” [27].

Our result Eq. (35) on the shape variation of F_θ is at variance with that of Ref. [16]. Using the Coulomb-gas model, the shape variation in this reference is done within conformal gauge, whereas the Coulomb-gas calculation of Sec. IV B is done in a general gauge. The result of Ref. [16], cast in our

notation, is

$$\frac{\delta F_\theta}{\delta R_\perp} = -2K_A H K, \quad (62)$$

as against our result Eq. (35). The full shape equation of Ref. [16] is

$$K_A K H + \sigma H = 0, \quad (63)$$

which, for nonzero H , implies that $K_A K + \sigma = 0$. The free energy F_θ couples gradients in the θ field to shape through the spin connection A . The most prominent difference between Eqs. (35) and (62) is that whereas Eq. (35) reflects this shape-order coupling via terms involving the stress function χ , Eq. (62) implies that the θ field is completely decoupled from the membrane-shape. In what follows we address the reason behind the discrepancy between our results and those of Ref. [16], before turning to their experimental implications.

To carry out the shape variation of a fluid membrane (with, or without orientational order), it is essential that the membrane surface be embedded in three-dimensional Euclidean space \mathbb{R}^3 . The fundamental theorem of surfaces [29,30] states that a surface embedded in \mathbb{R}^3 exists, and is uniquely specified (up to a Euclidean motion), if it has a first fundamental form (metric tensor), and a second fundamental form (curvature tensor) that satisfies Gauss-Codazzi equations. Merely specifying intrinsic properties of a surface such as the metric, and therefore the intrinsic curvature K , does not embed the surface in \mathbb{R}^3 .

In Ref. [16], it is assumed that the membrane is free of disclinations. The elastic free energy F_θ is written in conformal coordinates $\underline{u} = (u^1, u^2)$ by using the standard formula $K = -[1/(2w)] \partial_{\underline{u}}^2 \ln w$ for the Gaussian curvature, where w is the conformal weight, and $\partial_{\underline{u}}^2$ is the Euclidean Laplacian. It is then assumed that *all the geometrical structure of the interface (membrane) is embodied in the conformal weight $w(\underline{u})$* . We note that given the conformal metric alone, without specifying an associated extrinsic curvature tensor K_{ij} that satisfies Gauss-Codazzi equations, there is no notion of a unit normal \hat{n} to the surface. Therefore the interface considered in Ref. [16] is not embedded in \mathbb{R}^3 . In Ref. [16], the shape variation of F_θ is then carried out by using $\delta w = -2H w \delta R_\perp$ by analogy with the standard result $\delta \sqrt{g} = -2H \sqrt{g} \delta R_\perp$ for an embedded surface, followed by the use of Green's identities. Using a simple example, we now show that this procedure is inconsistent, and leads to absurd results. Let us consider the "shape variation" of the conformal metric tensor. In conformal coordinates $g_{ij} = w \delta_{ij}$, thus $\delta g_{ij} = \delta w \delta_{ij} = -2H w \delta_{ij} \delta R_\perp$, whereas the known normal variation for an embedded surface is $\delta g_{\mu\nu} = -2K_{\mu\nu} \delta R_\perp$, Eq. (33). The calculation of Ref. [16] therefore accounts merely for the variation of the area element alone, culminating in the erroneous result Eq. (62).

We note that Ref. [16] ignores the term proportional to $(H - H_0)^2$ in the elastic free energy Eq. (1). For membranes with up-down symmetry, such as symmetric bilayer membranes, $H_0 = 0$. However, even for symmetric bilayer membranes the term proportional to H^2 cannot be ignored; it is of the same order in the number of derivatives as K and is not explicitly forbidden by symmetry considerations. Moreover, even if the coefficient κ of the H^2 term is taken to be zero to begin with, thermal fluctuations generate a nonzero κ of order $k_B T$ [31]. For typical lipid membranes κ is on the order of

$10 k_B T$ [32]. Ignoring the mean curvature squared term in the elastic free energy is therefore physically unacceptable. The class of nonminimal, hyperbolic interfaces with $K = -\sigma/K_A$ proposed as equilibrium shapes in Ref. [16] do not satisfy the full shape Eq. (38). Even after including the shape variation of the H^2 term, the result of Ref. [16] does not, to the lowest order, reduce to the approximate (noncovariant) nonlinear, hexatic von Kármán Eq. (15) of Ref. [4]. This further confirms that the result Eq. (62) for the shape variation of F_θ is erroneous.

As mentioned in Sec. IV A, the shape equation as well as the free boundary conditions simplify considerably for minimal surfaces. Analytical results such as those of Ref. [14] for defects in nematic membranes either assume that $\kappa = 0$, or treat minimal surfaces (the helicoid of Sec. IV C). Because of the complex nature of these equations, most problems dealing with the equilibrium shape and texture of membranes have to be addressed by using either numerical methods (including simulations) or variational ansätze.

We now discuss the experimental implications of the results of [16] as against those of our results. Disclination induced buckling is one of the most important predictions of the Nelson-Peliti formulation. Below certain critical values of κ/K_A , the approximate von Kármán Eq. (15) predicts disclination-induced buckling of a planar membrane into a cone (for a +1 disclination), and a saddle (for a -1 disclination) [4,5]. The predicted shapes of the cone as well as the saddle have a nonzero mean curvature. These buckled shapes cannot be obtained by using the shape equation of Ref. [16] *because mean curvature drops out of the shape equation*, Eq. (63), whereas the shape Eq. (38), solved numerically in conjunction with the compatibility condition Eq. (13), would directly give the numerically exact shape of the membrane and its texture for given κ/K_A . Experimentally, the buckling of spherical nematic vesicles into "rounded tetrahedra" has been observed and has been compared with results obtained by energy minimization using simulated annealing Monte Carlo method [7]. The equations of equilibrium obtained by us have experimentally testable consequences not only in the field of fluid membranes but also for smectic liquid crystals with in-plane orientational order [15]. In this reference we have used the solution for a helicoid obtained in Sec. IV C to predict dispersion asymmetry in smectic-C* liquid crystals.

VI. SUMMARY AND CONCLUSIONS

Elastic free-energy of membranes endowed with orientational order depends on the shape of the membrane as well as the orientational order. The Nelson-Peliti formulation [3] of membrane elasticity used in this paper emphasizes the interplay between the shape of the membrane and the topology of the orientational-order field on it.

Minimization of the membrane free energy involves independent variation of the orientational order while keeping the membrane shape unchanged, and vice versa. Whereas it is straightforward to vary the orientational order on a membrane with a fixed shape, it is not obvious how membrane-shape can be varied for a fixed configuration of the orientational-order field. In this paper, we have proposed a purely geometrical

method for carrying out such shape-variation via a generalization of the Lie-dragging procedure.

Using two different methods, we have minimized the Nelson-Peliti elastic free-energy with respect to membrane-shape to obtain the covariant shape equation. The first method is direct and involves a particular choice of gauge. We have shown that this choice of gauge is consistent with Lie dragging. In addition to the equation of bulk equilibrium (the shape equation), the direct method also leads to free boundary conditions (for membranes with an edge, or a boundary) derived in this paper. The second method employs the Coulomb-gas version of the Nelson-Peliti elasticity [4] and establishes that the shape equation obtained through the direct method does not depend on the particular choice of gauge. The shape equation derived by us, together with the compatibility condition (that replaces the Euler-Lagrange equation corresponding to the minimization of the orientational-order field) form the set of coupled, nonlinear differential equations of bulk equilibrium. Our results on the shape equation, together with associated free boundary conditions are new. These are essential for understanding equilibrium configurations (shape as well as texture) of membranes with orientational order, especially in experimental situations involving topological defects, and large shape-deformations.

As an illustrative example, we have obtained an exact solution to the coupled equations of bulk equilibrium for a helicoid. Based upon our recent work [15], which uses the exact solution for helicoids obtained in the present paper, we have proposed an experimental test of our results on membranes in the unusual setting of lamellar liquid crystals with in-plane order—asymmetry in the energetics of dispirations (topological defects in smectic- C^* liquid crystals) having strengths of equal magnitude but opposite signs.

Derivation of the shape equation for membranes endowed with orientational order has been attempted earlier [16]. We have discussed the root causes that lead to an erroneous result for the shape equation proposed in Ref. [16]. In this context we have pointed out that it is not possible to obtain the shape equation using abstract surfaces described *solely* in terms of internal coordinates. We have contrasted the experimental consequences of the shape equation of Ref. [16] with those of our result, known experimental results, and known theoretical predictions from numerical studies.

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